Optimal experiment design for discrimination in predictive microbiology models

I. Stamati1, F. Logist1, J.-P. Gauchi2, J. Van Impe1

1. BioTeC & OPTEC, Chemical Engineering Department, KU Leuven, W. de Croylaan 46, 3001 Leuven, Belgium – CPMF2 Cluster Predictive Microbiology in Foods www.cpmf2.be

2. Unit MIA (UR341), INRA, Domaine de Vilvert, 78352 Jouy en Josas, France

OBJECTIVE(S)

In the field of predictive microbiology, mathematical models play an important role for describing microbial growth, survival and inactivation. Often different models are available for describing the microbial dynamics in a similar way. However, the model that describes the system in the best way is desired. In this respect, optimal experiment design for model discrimination (OED-MD) is an efficient tool for discriminating among rival models.

METHODS

The idea is to use optimal experiment design to discriminate between available models. To this end, new experimental conditions are designed that maximize the difference between the predictions of the different models. The difference in the model predictions enables the selection of the model that fits more accurately the experimental data. There exist in literature several criteria which take this difference into account. In the current work, two different criteria are used, i.e., (i) the T12-criterion employed by Ucinski and Bogacka (2005) and (ii) the Schwaab-approach proposed by Schwaab et al. (2008). The first criterion performs discrimination in a simultaneous way whereas the second does it in a sequential manner. In contrast to a typical set of experiments at constant levels, the dynamic experiments designed in the current work enable the discrimination between two models in a cost and labor efficient way.

RESULTS

For describing the influence of temperature on the microbial growth rate there exist several models in predictive microbiology. Two of these models are the CTMI (Cardinal Temperature Model with Inflection (Rosso et al., 1993) and the aCTMI (adapted CTMI (Le Marc et al., 2002)). While the CTMI model assumes a one-phase linear relation between the square root of the growth rate and the temperature in the suboptimal temperature range, the aCTMI starts from the assumption of two phases in this temperature region. Up till now, it has been assumed that the CTMI is generally valid for E. coli K12. In this work, the possibility of discriminating between the CTMI and aCTMI models has been evaluated in silico.

First, preliminary experiments have been performed to yield parameter estimates which are good enough to start the model discrimination procedure. Afterwards both criteria have been exploited and found to provide dynamic temperature profiles capable of discriminating between the CTMI and aCTMI model. Although both approaches perform almost identically, the Schwaab-procedure yields less biased parameter estimates and requires less computational effort. Obviously, the T-procedure was not designed for obtaining good estimates whereas for the Schwaab-approach this appears to be the case.

CONCLUSIONS AND IMPACT OF THE STUDY

Based on the in silico study, the proposed experimental design methods for model discrimination can be used to evaluate if the diverging kinetics (observed for Listeria strains), also hold for E. coli K12. Hence, the above-mentioned discrimination methods provide an efficient way to select an appropriate predictive microbiology model with less experimental effort.

REFERENCES

Le Marc et al. 2002. Modeling the growth kinetics of listeria as a function of temperature, pH and organic acid concentration. International Journal of Food Microbiology 73, 219–237.

Rosso et al. 1993. An unexpected correlation between cardinal temperatures of microbial growth highlighted by a new model. Journal of Theoretical Biology 162, 447–463.

Schwaab et al. 2008. Sequential experimental design for model discrimination. taking into account the posterior covariance matrix of parameter uncertainties. Chemical Engineering Science 63, 2408–2419.

Ucinski and Bogacka. 2005. T-optimum designs for discrimination between two multiresponse dynamic models. Journal of the Royal Statistical Society 67, 3–18.